

Dissipation due to two-level systems in nano-mechanical devices

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Abstract. - We analyze the dissipation of the vibrations of nano-mechanical devices. We show that the coupling between flexural modes and two-level systems leads to sub-ohmic dissipation. The inverse quality factor of the flexural modes of low frequencies depends on temperature as $Q^{-1}(T) \approx Q_0 + CT^{1/3}$, providing a quantitative description of the experimental data.

Introduction. – Nano-electro-mechanical devices [1, 2] (NEMS) are systems with great potential for applied physics and engineering because of their extreme sensitivity, as probes, to their environment [3–9]. Furthermore, because of their small size and large surface to volume ratio, these systems are in the crossover region between classical and quantum behavior, and hence of great theoretical interest. Thus, the study of the sources of noise and dissipation in these systems has attracted a great deal of attention [10–18]. One of the common realizations of nano-mechanical resonators is a rigid beam of nanoscopic dimensions which vibrates at GHz frequencies [19,20]. The damping of these oscillations has been a subject of intense investigation [10,13,15,16], as it sets a limit to their possible applications.

The damping of a low frequency oscillation in a NEMS comes from the coupling of this mode to other low energy degrees of freedom. Experiments suggest that surfaces of nano-mechanical resonators resemble amorphous bulk systems [21], with a high density of defects, playing a major role as a source of dissipation [22]. In amorphous solids, disorder and impurities lead to the existence of anharmonic excitations, which can be modeled as a degree of freedom tunneling between two potential wells [23]. A simpler two-level system (TLS) description arises at low temperatures, when only the two lowest eigenstates have to be considered. Some properties of the distribution of TLSs in terms of their parameters (bias, Δ_0^z , and tunneling rate, Δ_0^x) can be inferred from experiments [24], and they are considered to be the main source of damping of acoustical modes in disordered insulating solids [24–27].

In this work, we study mostly a rigid beam geometry, sketched in fig. [1], and analyze the dissipation processes for low energy flexural modes due to the presence of effective TLSs at its surface. The generalization to dissipation of torsional modes is straightforward and will be given elsewhere. Once a given mode is externally excited, the TLSs living at the surface of the beam, which are coupled to this mode, will absorb part of its energy. But as the TLSs are also coupled to the rest of vibrational modes of the beam, they will release most of this energy to them. Thus the TLSs give rise to an indirect coupling between the externally excited mode and the rest of modes. For the experimentally relevant case of low amplitudes of vibration this coupling prevails over the usual anharmonic coupling.

This energy flow process will be described in two stages:

i) From the point of view of a given TLS, its coupling to the vibrational modes of the beam, which can be seen as an external bath, alters its dynamics and enables it to absorb and emit energy in a broad range of frequencies. In particular, the presence of flexural modes leads to the possibility of qualitative changes in the dynamics of the TLSs, as the former constitute a *sub-ohmic* environment [28, 29] for the TLSs. This is a consequence of the quadratic dispersion relation characteristic of flexural modes, which results in an enhancement of the density of low frequency modes.

ii) Coming back to the externally excited vibrational mode whose damping we want to compute, the TLSs, dressed by all the vibrational modes of the structure, constitute the dissipative environment for the mode. This

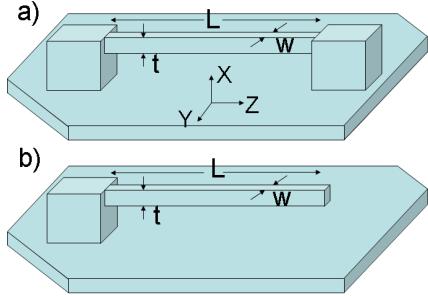


Fig. 1: Sketch of the NEMS: a) Doubly clamped beam, suspended by both ends; b) Cantilever, with one free end. The device is characterized by its width (w), thickness (t), and length, (L), where $w \sim t \ll L$.

involves TLSs that are nearly resonant with the mode under consideration but also off resonance TLSs since the strong phonon/TLS coupling provides each TLS spectral function with tails far from resonances. In many NEMS experiments, the flexural modes studied are highly excited, either because of an external driving mechanism, or because the temperature is much higher than the frequency of the mode. As a given TLS can absorb and emit over a broad range of energies, due to the incoherent tails in its spectrum (see below), these processes allow for the transfer of energy from a highly excited low frequency flexural mode to other modes with higher frequencies.

Dissipative mechanisms other than TLSs, which have been extensively studied elsewhere [30–32], are not considered here.

TLSs coupled to low dimensional vibrations. –

The TLSs are mainly coupled to the strain induced by phonons. It is assumed that the main effect of the strain is to modify the energy splitting between the TLSs energy levels [33]. The Hamiltonian of a given TLS is characterized by a bias, Δ_0^z , and the tunneling rate, Δ_0^x (we use units such that $\hbar = 1 = k_B$, and omit the part of the Hamiltonian describing free vibrations):

$$H = \Delta_0^x \sigma_x + \Delta_0^z \sigma_z + \sigma_z F(\partial_i u_j) \quad (1)$$

where $\partial_i u_j$ is a component of the deformation gradient matrix, and F is an arbitrary function. Changing basis to the energy eigenstates of the TLS, eq.(1) becomes $H = \Delta_0 \sigma_z + [(\Delta_0^x / \Delta_0) \sigma_x + (\Delta_0^z / \Delta_0) \sigma_z] F(\partial_i u_j)$. $\Delta_0 = \sqrt{(\Delta_0^x)^2 + (\Delta_0^z)^2}$ is the splitting of the TLS. Dissipation is dominated by slightly biased TLSs for whom $\Delta_0^z \ll \Delta_0$, so the last term can be ignored. A further expansion of F to lowest order in the displacement, together with a $\pi/4$ rotation of the eigenbasis, leads to: $H = \Delta_0 \sigma_x + \gamma (\Delta_0^x / \Delta_0) \sigma_z \partial_i u_j$, where γ is the coupling constant (with dimensions of energy).

The main interaction between phonons and TLSs is due to the coupling to the operator σ_z of each TLS. Hence, the absorption properties of each TLS can be characterized by

the spectral function:

$$A(\omega) \equiv \sum_n |\langle 0 | \sigma_z | n \rangle|^2 \delta(\omega - \omega_n + \omega_0) \quad (2)$$

where $|n\rangle$ is an excited state of the total system TLS plus vibrations. The linearization of the coupling implies that the interaction between a given TLS and the vibrations can be written as $H_{int} \equiv \sigma_z \sum_k \lambda_k (b_k^\dagger + b_k)$.

We also define a spectral function that determines the damping induced by phonons on the TLS: $J(\omega) \equiv \sum_k |\lambda_k|^2 \delta(\omega - \omega_k)$ where ω_k is the energy of mode k . The vibrational modes of a beam with fixed ends have a discrete spectrum, but we will approximate them by a continuous distribution. This approximation will hold as long as many vibrational modes become thermally populated, $kT \gg \hbar \omega_{fund}$, where ω_{fund} is the frequency of the lowest mode. The condition is fulfilled in current experimental setups.

Acoustic modes of a nanoscopic beam. Using continuum elasticity theory [34], a one-dimensional (1D) rod has compression and twisting modes, with a linear relation between frequency and momentum, and bending, or flexural, modes, where the frequency depends quadratically on momentum. We will consider a rod of length L , width w and thickness t , see Fig.1]. We describe next the spectral function which describes how the modes of the rod absorb energy in different energy ranges.

The compression and twisting modes lead to an ohmic spectral function for $\omega \ll 2\pi c/R$ (R being a typical transversal dimension of the rod and c the sound velocity), when the rod is effectively 1D. In terms of the Young modulus of the material, E , and the mass density, ρ , we get: $J_{comp}(\omega) = \alpha_c |\omega|$, where,

$$\alpha_c = (\gamma \Delta_0^x / \Delta_0)^2 (2\pi^2 \rho t w)^{-1} (E/\rho)^{-3/2}. \quad (3)$$

The twisting modes are defined by the torsional rigidity, $C = \mu t^3 w / 3$ (μ is a Lande coefficient), and $I = \int dS x^2 = t^3 w / 12$ (where S is the cross-section). The corresponding spectral function is given by: $J_{torsion}(\omega) = \alpha_t |\omega|$, where

$$\alpha_t = C (\gamma \Delta_0^x / \Delta_0)^2 (8\pi^2 \mu t w \rho I)^{-1} (\rho I / C)^{3/2}. \quad (4)$$

The analysis of the flexural (bending) modes differs substantially from the other ones, because they correspond to two fields $\Phi_j(z, \omega)$ ($j = x, y$) that satisfy [34]: $E I_j \partial_z^4 \Phi_j = \rho t w \omega_j^2 \Phi_j$, where, for the system considered here, $I_j = t^3 w / 12$. The normal modes have a quadratic dispersion $\omega_j(k) = \sqrt{E I_j / (\rho t w)} k^2$. Their corresponding spectral function is sub-ohmic [28], $J_{flex}(\omega) = \alpha_b \sqrt{\omega_{co}} \sqrt{\omega}$, with,

$$\alpha_b \sqrt{\omega_{co}} = 0.3 \frac{\gamma^2}{t^{3/2} w} \frac{(1 + \nu)(1 - 2\nu)}{E(3 - 5\nu)} \left(\frac{\rho}{E} \right)^{1/4}, \quad (5)$$

where ν is Poisson's ratio and $\omega_{co} \simeq \sqrt{E I_y / (\rho t w)} (2\pi/t)^2$ is the high energy cut-off of the bending modes. Collecting the previous results, we find the spectral function $J(\omega)$ plotted in Fig.[2].

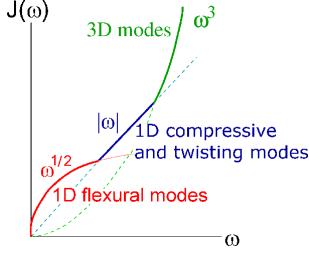


Fig. 2: Sketch of the contributions to the spectral function which determines the dynamics of the TLS.

Dynamics of the TLSs. – We are interested in the TLSs that affect most the low-energy flexural vibrations. Hence, we focus on the TLSs whose tunneling amplitudes lie in the region where the damping is sub-ohmic. We define Δ_r as the tunneling amplitude of a given TLS, including the renormalization due to the high energy acoustic modes. We assume, as in the case of glasses, that the distribution of these TLSs is given by [24, 25] $g(\Delta_r, \Delta_z) = P/\Delta_r$. The sub-ohmic coupling, eq.(5), leads to a renormalization of Δ_r :

$$\Delta_{ren} = \Delta_r \exp\left\{-\alpha_b \sqrt{\omega_{co}} \int_{\Delta_{ren}}^{\omega_{co}} d\omega J(\omega)/\omega^2\right\} \quad (6)$$

This equation has no solutions other than $\Delta_{ren} = 0$ if $\Delta_r \ll \alpha_b^2 \omega_{co}$, so that the tunneling amplitude of the low energy TLSs is strongly suppressed [28, 29, 35, 36]. The remaining TLSs experience a shift and a broadening of the spectral function function $A(\omega)$, defined in eq.(2). In addition, $A(\omega)$ acquires a low energy tail, which, at zero temperature, is [37]:

$$A(\omega) \propto \alpha_b \frac{\sqrt{\omega_{co}\omega}}{\Delta_{ren}^2} \quad \omega \ll \Delta_{ren} \quad (7)$$

There is also a high energy part, $A(\omega) \propto \alpha_b \sqrt{\omega_{co}} \Delta_{ren}^2 \omega^{-7/2}$, for $\omega \gg \Delta_{ren}$. The main features of $A(\omega)$ are shown in fig. [3]. Finally, we obtain the width of the resonant peak, $\Gamma(\Delta_{ren})$, using Fermi's golden rule, $\Gamma(\Delta_{ren}) = 16\alpha_b \sqrt{\omega_{co}} \sqrt{\Delta_{ren}}$. This description is valid for wavelengths such that, $1/L \ll k \ll 1/\max(w, t)$.

The value of Δ_z is not renormalized by the phonons, so that the TLS cannot exchange energy with the environment at frequencies lower than Δ_z . In the following, we will consider only TLSs with $\Delta_z \lesssim \Delta_{ren}$.

The total absorption rate by the ensemble of dressed TLSs present in the beam, $A_{tot}(\omega)$, is obtained summing over $g(\Delta_r, \Delta_z)$ the values of $A(\omega)$, eq.(2), of each dressed TLS. In amorphous insulators, like amorphous silica, there are TLSs with Δ_r up to about $\omega^* = 5$ K [24]. The upper cut-off of the distribution is usually larger than the frequencies of the flexural modes of interest, $\omega_{co} < \omega^*$. Integrating over Δ_z and Δ_{ren} , we find that the density of TLSs per unit volume and unit energy available for direct (resonant) excitation processes is given by P , in

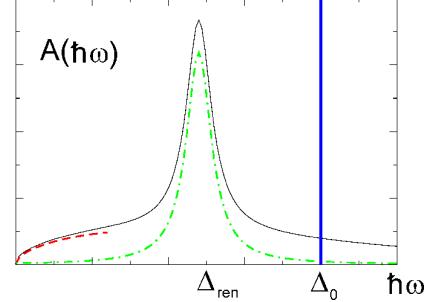


Fig. 3: Sketch of the spectral function of a TLS coupled to a sub-ohmic bath. Dashed line shows the off-resonant contribution. Dot-dashed line shows the main broadened peak. For comparison, the thick vertical line shows the spectral function of a non-interacting TLS.

agreement with the known result that TLSs in amorphous systems give rise to a finite density of states at low energies [25]. In addition, we find a contribution coming from the non-resonant part of the spectral function of each TLS, $A_{tot}^{off-res}(\omega) \approx 2P\alpha_b \sqrt{\omega_{co}/\omega}$. The divergence as $\omega \rightarrow 0$ arises from the Δ_{ren}^{-2} dependence of $A(\omega)$, eq.(7).

Dissipation due to the TLSs. – We assume that the externally excited flexural mode of interest, (k_0, ω_0) , is linearly coupled, with the coupling constant shown in the derivation of the hamiltonian H , $\gamma(\Delta_0^x/\Delta_0)$, to a continuum of excitations whose spectral strength, $A_{tot}(\omega)$, is given by the summation over all TLSs of the function $A(\omega)$ calculated for each one. The ratio (Δ_0^x/Δ_0) can be approximated as 1, due to the negligible role played by strongly biased TLSs.

The transition rate of the mode k_0 occupied by n phonons to the mode with $n-1$ is calculated from Fermi's golden rule, and the energy loss per cycle and unit volume ΔE of the mode will correspond to this transition rate multiplied by the energy of a phonon $\hbar\omega_0$ and the period $2\pi/\omega_0$:

$$\Delta E \simeq \frac{2\pi}{\omega_0} \times \hbar\omega_0 \times \frac{2\pi}{\hbar} n \left(\gamma \frac{k_0^2}{\sqrt{\omega_0}} \right)^2 A_{tot}(\omega_0) \quad (8)$$

where $A_{tot}(\omega) = P + P\alpha_b \sqrt{\omega_{co}/\omega}$ is the sum of the resonant and non resonant contributions arising from integrating over the distribution of TLSs, as discussed in the preceding paragraph.

The inverse quality factor $Q^{-1}(\omega_0)$ is given by $Q^{-1}(\omega_0) = \Delta E/2\pi E_0$, where E_0 is the energy stored in the mode per unit volume, $E_0 \simeq n\hbar\omega_0/twL$, leading to the following expression at zero temperature:

$$Q^{-1}(\omega_0) \simeq 10t^{3/2}w \left(\frac{E}{\rho} \right)^{1/4} \alpha_b \sqrt{\omega_{co}} A_{tot}(\omega_0) \quad (9)$$

Experiments are done at finite temperatures, and, sometimes, in systems where the oscillator is driven strongly

out of equilibrium. We take these effects into account by calculating $A_{tot}(\omega, T)$ in the presence of a finite distribution of excited vibrations, which can include a non-thermal contribution. If we only keep one phonon processes in the calculation of $A_{tot}(\omega, T)$, as in the previous discussion, the subtraction of absorption and emission processes cancel the temperature dependence on the number of phonons. The only temperature dependence is due to saturation effects in the absorption properties of the TLSs when their environment contains many quanta of energy Δ_{ren} . The final expression for the inverse quality factor at finite temperatures is:

$$Q^{-1}(\omega_0, T) \simeq 10t^{3/2}w \left(\frac{E}{\rho}\right)^{1/4} \alpha_b \sqrt{\omega_{co}} \times \\ \times \left[P \tanh\left(\frac{\hbar\omega_0}{k_B T}\right) + P \alpha_b \sqrt{\frac{\omega_{co}}{\omega_0}} \right] \quad (10)$$

Until now prevalence of one-phonon processes in the interaction among TLSs and vibrational modes has been assumed, but at temperatures much higher than the frequencies of the relevant phonons, multi-phonon processes need to be taken into account. We include this effect assuming overdamped dynamics for the TLSs, so that $A(\omega, \Delta_{ren}, T) = \tau(\Delta_{ren}, T)/(1 + [\omega\tau(\Delta_{ren}, T)]^2)$, where $\tau(\Delta_{ren}, T) = \Gamma^{-1}(\Delta_{ren}, T)$, and making use of the relation between $Q^{-1}(\omega, T)$ and $A(\omega, \Delta_{ren}, T)$ usually found in the context of the standard tunneling model approach to disordered bulk systems [24–27, 38], which in our case translates into:

$$Q^{-1}(\omega, T) = P\gamma^2/(ET) \int_0^{\epsilon_{max}} d\epsilon \int_{u_{min}}^1 du \sqrt{1-u^2}/u \times \\ \times \frac{\cosh^{-2}(\frac{\epsilon}{2T}) \omega\tau}{1 + (\omega\tau)^2} \quad (11)$$

Here $\epsilon = \sqrt{\Delta_{ren}^2 + \Delta_z^2}$ and $u = \Delta_{ren}/\epsilon$, with u_{min} fixed by the time needed to obtain a spectrum around the resonance frequency of the excited mode and ϵ_{max} estimated to be at least of the order of 5 K [24]. The limits of integration must be such that only the overdamped TLSs are included. A given TLS is overdamped when $\Delta_{ren} \leq \Gamma(\Delta_{ren}, T) \rightarrow \Delta_{ren} \leq [30\alpha_b \sqrt{\omega_{co}T}]^{2/3}$. Hence, we obtain for the contribution to the inverse quality factor from overdamped TLSs:

$$Q^{-1}(\omega_0, T) \approx \frac{400P\gamma^2(\alpha_b \sqrt{\omega_{co}})^{4/3} T^{1/3}}{E\omega_0} \quad (12)$$

Therefore, in a range of energies $\omega_{fund} \leq \omega_0 \ll \omega_{co}$, the attenuation coming from these TLSs shows a $Q^{-1}(T) \sim T^{1/3}$ dependence, in qualitative agreement with the experiment [18] on Si nanobridges. The total inverse quality factor is the sum of eq.(12) plus the temperature independent contribution arising from off-resonant processes induced by underdamped TLSs, eq.(10). This last equation must in principle be corrected by taking into account the decrease

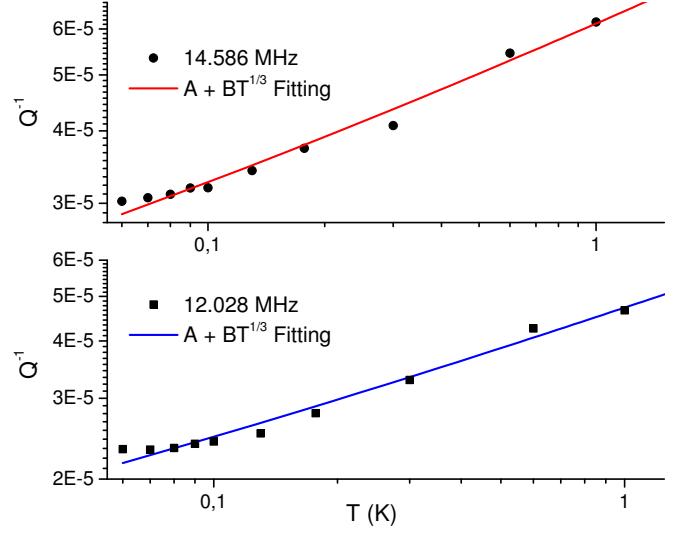


Fig. 4: Fittings of the result of eq.(13) to experimental data [18].

in the number of underdamped TLSs as the temperature is raised, but it is a weak effect and will be neglected, leading to the final expression for the total attenuation of a flexural mode:

$$Q^{-1}(\omega_0, T) \sim Q_0^{-1}(\omega_0) + C(\omega_0)T^{1/3}, \quad (13)$$

where,

$$Q_0^{-1}(\omega_0) \simeq \frac{3P\gamma^4\rho^{1/4}}{t^{3/2}wE^{9/4}} \left[\frac{(1+\nu)(1-2\nu)}{3-5\nu} \right]^2 \omega_0^{-1/2} \\ C(\omega_0) \simeq \frac{150P\gamma^4\rho^{1/3}}{t^2w^{4/3}E^4\omega_0} \left[\frac{(1+\nu)(1-2\nu)}{3-5\nu} \right]^{4/3} \quad (14)$$

As only part of the beam is amorphous, P is to be replaced by $P \cdot V_{\text{amorphous}}/V_{\text{total}}$. To describe the results in [18], as shown in fig. [4], we assumed $P \cdot V_{\text{amorphous}}/V_{\text{total}} \sim 10^{44} \text{ J}^{-1} \text{ m}^{-3}$, compatible with P values reported in amorphous glasses [24], and $0.1 \lesssim V_{\text{amorphous}}/V_{\text{total}} \lesssim 1$. The slope of the $T^{1/3}$ contribution gives the value of γ , used as fitting parameter. We obtain $\gamma \sim 5 - 10 \text{ eV}$, which is a reasonable value [39, 40]. There are two limitations on the range of applicability of our results. The increasing role of interactions between TLSs as T is lowered [41], and possible cooperative effects when the mode is strongly driven [16] cause deviations, which are manifested in the saturation observed in fig.(4), not explained by our fit, which predicts $Q_0^{-1} \sim 5 \cdot 10^{-7}$. On the high-temperature side, a point is reached when the rate $\Gamma^{-1}(\Delta_{ren}, T)$ changes to an Arrhenius-like behavior [24].

Conclusions. – We have studied the damping of mechanical oscillations in nanoscopic devices due to their interaction with TLSs. This coupling is the main mechanism of relaxation of phonons in disordered insulators. We have analyzed the changes induced in the spectrum and

distribution of TLSs due to their interaction with the low energy oscillations of nano-mechanical devices. Flexural modes, with a high density of states at low energies, lead to sub-ohmic damping, which can modify significantly the distribution of TLSs. The problem of a TLS interacting with a sub-ohmic environment is interesting in its own right [28, 29, 36, 42–48], and the systems studied here provide a physical realization.

We obtain a temperature independent contribution to the inverse quality factor, Q^{-1} of a flexural mode, which arises from resonant excitations of TLSs, and off-resonant processes involving underdamped TLSs. We find, in addition, a contribution which increases as $T^{1/3}$, arising from overdamped TLSs. The off-resonant contributions imply that the externally excited vibration loses its energy to TLSs which, in turn, decay into other acoustic modes. Hence, off-resonant contributions can only be present if the number of thermally excited modes is large, a situation fulfilled in most present experiments.

We have made numerical estimates for the expected dissipation for a few representative devices. We have assumed that a fraction of the device shows amorphous features, and contains a distribution of TLSs similar to that found in amorphous insulators. The main uncertainties in our calculation are due to the lack of information on the TLSs distribution, the coupling strength, and the fraction of the total volume of the device that they occupy. Decreasing volume and number of modes may lead as well to fluctuations around our predictions, which use continuum distributions.

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